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PLUME MECHANICS AND PARTICLE GROWTH PROCESSES.

FINAL REPORT

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J. R. BROCK

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Numerical models have been developed for studying aerosol growth processes in dispersing smoke plumes. The principal growth processes are coagulation and condensation/evaporation. For coagulation, the existence of asymptotic limit distributions has been demonstrated. It is shown that the condensation/evaporation process can lead to multimodal particle size distributions. The aerosol growth processes have been incorporated in a general K-theory model for dispersion of smoke plumes. Some of the results from field measurements of plumes from

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smoke munitions support conclusions based on our numerical model studies.

Objectives of Research

Work under this grant was intended to add to the technological base of the U.S. Army's smoke program as well as to contribute to fundamental knowledge of aerosol physics. In this study, the principal focus has been on the influence of smoke plume/puff dispersion on aerosol growth.

Aerosol growth processes and dispersion determine the particle size and composition distributions. These distributions dictate the obscuration efficiency of smoke plumes/puffs. As a smoke plume/puff disperses, the dispersion process itself will affect the principal smoke particle growth processes--coagulation and condensation/evaporation. Our aim has been to understand and incorporate these growth processes at realistic particle number concentrations into a K-theory model for plume dispersion.

Summary of Results

The particle size and composition distributions in a dispersing smoke plume/puff determine the obscuration efficiency of a smoke material. These distributions are produced by a number of complex aerosol growth and transport processes, as well as by the dispersion process itself. Completely rigorous descriptions of many of the aerosol growth processes do not yet exist. Consequently, work on the subject grant was initiated by a critical review, subsequently published (1), of the kinetics of ultrafine particles. This review has had an

important influence on our development of models for aerosol growth and transport.

This summary gives the important findings of our research into the relationships between smoke particle growth and dispersion. First, numerical studies of the coagulation process are described. Principal results from similar studies of the condensation/evaporation process are then presented. Finally, important aspects of a general K-theory incorporating these growth processes are described along with characteristics of particle size distributions observed in a smoke munitions field test.

Coagulation

The following results have been obtained during the course of coagulation studies under this grant.

1) The singlet density function, $n(x,t)$ plays an important role in many aerosol applications. Here $n(x,t)dx$ represents the number of particles which at time t have masses in the interval x,dx. We have demonstrated that the equation for the evolution of $n(x,t)$ by Brownian coagulation

$$\frac{\partial n(x,t)}{\partial t} = \int_0^{x/2} b(x-x',x')n(x-x',t)n(x',t)dx'$$

$$- n(x,t) \int_0^{\infty} b(x,x')n(x')dx' \qquad (1)$$

can be solved numerically for initial multimodal density functions covering the order of three decades of particle

diameter with total particle concentrations as large as $10^{15}cm^{-3}$. In our calculation procedure, a logarithmic transformation of x-space is used. The error in the numerical solution of Eq. (1) can be reduced as desired by increasing the number of logarithmic intervals. For the simulation of growth of typical condensation aerosols with error in total mass maintained at the 2% level, the average computation time per time step is in the range of 1×10^{-5} to 1×10^{-3} octal seconds, the largest time being required for initial total particle concentrations of $10^{15}cm^{-3}$. The computer code has been made available to personnel of the Chemical Systems Laboratory, Aberdeen Proving Ground.

2) It has been shown (2) that the Brownian coagulation equation (1) with the expression for $b(x,x')$ due to Fuch (1) possesses an asymptotic limit distribution (ALD) which is independent of the form of the initial density function, $n(x,t=0)$. This has been confirmed (2) for the non-dimensional form of Eq. (1) with the following initial distribution functions: log-normal gamma, first-order gamma, log-gamma, beta of second kind, triangular, rectangular, and power law (Junge-type). By three measures of goodness of fit (spectral, Smirnoff and Kolmogoroff) and five test distributions (log-normal, gamma, first-order gamma, log-gamma and

beta of second kind) the log-gamma distribution was found to give the best fit of the Brownian ALD.

Condensation/Evaporation

In order to develop numerical methods for describing the evolution of an aerosol in dispersing plumes/puffs, we have also investigated several aspects of the evolution of n(x,t) by condensation/evaporation processes. Some important results of this part of the research are as follow.

1) Efficient computer codes have been developed for numerical solution of the equations for the evolution of n(x,t) by condensation. These equations have the form:

$$\frac{\partial n(x,t)}{\partial t} = - \frac{\partial}{\partial x} [\psi(x,t)n(x,t)] \tag{2}$$

which is coupled through the condensation/evaporation rate ψ to the mass density $S_{j\infty}$ of the condensing vapor:

$$\frac{\partial S_{j\infty}}{\partial t} = \nu_j - {}_o\int^{\infty}\psi(x,t)n(x,t)dx \tag{3}$$

ν_j represents possible sources or sinks (other than condensation) of vapor. The condensation/evaporation rate $\psi(x,t)$ has the form (3):

$$\psi(x,t) = (3x/4\pi\rho_p)^{2/3}\bar{v}_j S_{jo}\left(\frac{S_{j\infty}}{S_{jo}} - e^{\kappa/R_p}\right)\cdot F(Kn)$$

F(Kn) is a function of Knudsen number whose form is known only approximately (3,4). ρ_p is the mass density

of a particle. $\bar{v}_j$ is the mean molecular speed of vapor molecule j and $S_{j\infty}$ is the vapor mass concentration at a large distance from a particle; the quasi-single particle regime is assumed (4). S_{jo} is the mass density at the particle surface arising from the vapor pressure of a plane surface. κ is the Kelvin coefficient in the exponential term which allows for the effect of radius of curvature R_p on the vapor pressure (3,4). Equations (2) and (3) provide simulations of evolution of smokes by condensation/evaporation as in closed chamber experiments commonly used to study obscuration. The computer code for numerical solution of Eqs. (2) and (3) has been made available to personnel of Chemical Systems Laboratory, Aberdeen Proving Ground. This code has also been combined with that for coagulation (Eq. (1)) and has subsequently been included in a general plume dispersion model.

2) It has been shown (5,6) that under fairly general conditions, an initial unimodal density function evolves by Eqs. (2) and (3) into multimodal density functions. Bimodal density functions for oil smokes have been observed both in chamber experiments at Chemical Systems Laboratory as well as in the field at the U.S. Army Smoke Week III (7). These observations and these numerical results are also supported by controlled experiments following the evolution of condensation oil aerosols in a laminar coaxial jet, which was supported by a companion ARO research grant (8).

Aerosol Evolution in Dispersing Smoke Plumes

An understanding of aerosol evolution in dispersing plumes is a necessary step in the development of more efficient obscuration smokes. As a contribution to this, the following work has been carried out:

1) We have developed numerical methods (9) for incorporating aerosol growth processes into an atmospheric K-theory dispersion model (10), as depicted by the equation

$$\partial n(x;\vec{r},t)/\partial t + \vec{U}\cdot\nabla n(x;\vec{r},t) = \nabla\cdot\bar{\bar{K}}\cdot\nabla n(x;\vec{r},t) + \vec{G}(x)\cdot\nabla n(x;\vec{r},t)$$

$$+ \int_0^{x/2} b(x-x';x')\,n(x-x';\vec{r},t)\,n(x';\vec{r},t)\,dx'$$

$$- n(x;\vec{r},t)\int_0^{\infty} b(x,x')\,n(x';\vec{r},t)\,dx' - \frac{\partial}{\partial x}\left[\psi n(x;\vec{r},t)\right] \qquad (4)$$

with appropriate bounding conditions, including dry deposition. Eq. (4) is coupled to conservation equations for those chemical species undergoing condensation/evaporation. In Eq. (4), $\vec{U}$ is the mean wind velocity, $\bar{\bar{K}}$ the eddy diffusivity tensor and $\vec{G}(x)$ is the particle sedimentation velocity. The justification for a K-theory treatment of aerosol evolution in the ambient atmosphere has been given previously (10).

Under appropriate meteorological conditions (9), Eq. (4) permits for the first time detailed study of aerosol evolution in dispersing plumes. Such study can clearly lead to improved obscuration smokes.

2) A new fast response instrument (termed the ECI) for measuring aerosol size distribution (11) has been used to monitor dispersing smoke plumes from U.S. and foreign munitions at trials held at Smoke Week III, 4-22 August 1980, Elgin Air Force Base, Florida. In a number of smoke trials, bimodal number distributions were found. In a few trials, relatively large numbers of particles were found in the size range 0.01-0.25 μm (7).

Publications and Technical Reports

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2. Yom, K. S. and Brock, J. R., "Asymptotic Limit Distributions for Brownian Coagulation," Submitted for publication.

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Participating Scientific Personnel

1. K. S. Yom, PhD Candidate (Degree expected, May 1981).
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3. Dr. S. H. Baek (Postdoctoral research associate).
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